

4,5-Dibromo-1-methyl-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)-1H-pyrrole-2-carboxamide
113589-14-3 | DTXSID20556731

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.90e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.53e-01

Confidence level: 5.87e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Benomyl</div> <div>Measured: 1.31e-05</div> <div>Predicted: 3.43e-03</div>	<div>Image not found</div> <div>Mebendazole</div> <div>Measured: 2.41e-04</div> <div>Predicted: 3.12e-04</div>	<div>Image not found</div> <div>Thiophanate-methyl</div> <div>Measured: 7.77e-05</div> <div>Predicted: 3.83e-04</div>
<div>Image not found</div> <div>N-2-naphthylimidodicarbonimidic diamide</div> <div>Measured: 2.82e-03</div> <div>Predicted: 3.29e-03</div>	<div>Image not found</div> <div>1-(diaminomethylidene)-2-naphthalen-1-ylguanidine</div> <div>Measured: 4.84e-03</div> <div>Predicted: 7.15e-03</div>	